10/681,427

```
=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 13:54:28 ON 14 JUL 2004
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FILE COVERS 1907 - 14 Jul 2004  VOL 141 ISS 3
FILE LAST UPDATED: 13 Jul 2004  (20040713/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


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=> d stat que
L11             STR
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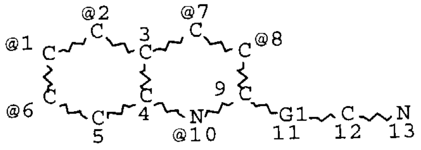

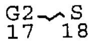

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REP G1=(0-10) C
VAR G2=1/2/6/7/8/10
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  15

STEREO ATTRIBUTES: NONE
L13            72 SEA FILE=REGISTRY SSS FUL L11
L14               STR
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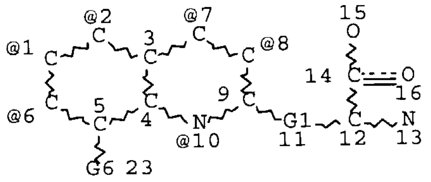

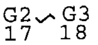

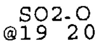

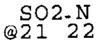

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REP G1=(1-4) C
VAR G2=1/2/6/7/8/10
VAR G3=19/21
VAR G6=OH/N/S
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  23

STEREO ATTRIBUTES: NONE
L15             3 SEA FILE=REGISTRY SUB=L13 SSS FUL L14
L16             2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L15



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=> d ibib abs hitrn l16 1-2

L16  ANSWER 1 OF 2  HCAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:        2003:861236  HCAPLUS Full-text
DOCUMENT NUMBER:         140:55461
TITLE:                   Versatile Fluorescence Probes of Protein Kinase
                         Activity
AUTHOR(S):               Shults, Melissa D.; Imperiali, Barbara
CORPORATE SOURCE:        Department of Chemistry and Department of Biology,
                         Massachusetts Institute of Technology, Cambridge, MA,
                         02139, USA
SOURCE:                  Journal of the American Chemical Society (2003),
                            125(47), 14248-14249
                            CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER:                  American Chemical Society
DOCUMENT TYPE:              Journal
LANGUAGE:                   English
AB     We introduce a versatile fluorescent peptide reporter of protein kinase activity.
       The probe can be modified to target a desired kinase by changing the kinase
       recognition motif in the peptide sequence.  The reporter motif contains the Sox
       amino acid, which generates a fluorescence signal when bound to Mg2+ present in the
       reaction mixture  The phosphorylated peptide exhibits a much greater affinity for
       Mg2+ than its unphosphorylated analog and, thus, a greater fluorescence intensity.
       Product formation during phosphorylation by the kinase is easily followed by the
       increase in fluorescence intensity over time.  These probes exhibit a 3-5-fold
       increase in fluorescence intensity upon phosphorylation, the magnitude of which
       depends on the substrate.  Peptides containing the reporter functionality are
       phosphorylated on serine by Protein Kinase C and cAMP-dependent protein kinase and
       are shown to be good substrates for these enzymes.  The principle of this design
       extends to peptides phosphorylated on threonine and tyrosine.
IT     639079-38-2
      RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical
      study); BIOL (Biological study)
         (versatile continuous fluorescence assay for protein kinase activity
         using Sox amino acid-containing peptide)
REFERENCE COUNT:            22      THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS
                                    RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16  ANSWER 2 OF 2  HCAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:           2003:617587  HCAPLUS Full-text
DOCUMENT NUMBER:            139:300801
TITLE:                      Modular and Tunable Chemosensor Scaffold for Divalent
                            Zinc
AUTHOR(S):                  Shults, Melissa D.; Pearce, Dierdre A.; Imperiali,
                            Barbara
CORPORATE SOURCE:           Department of Chemistry, Massachusetts Institute of
                            Technology, Cambridge, MA, 02139, USA
SOURCE:                     Journal of the American Chemical Society (2003),
                            125(35), 10591-10597
                            CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER:                  American Chemical Society
DOCUMENT TYPE:              Journal
LANGUAGE:                   English
AB     A modular peptide scaffold was developed for fluorescent sensing of divalent zinc.
       The signaling component of the chemosensor is the chelation-sensitive fluorophore 8-
       hydroxy-5-(N,N-dimethylsulfonamido)-2- methylquinoline, which is prepared as the
       protected amino acid derivative Fmoc-Sox-OH and integrated into peptide sequences.
       Nineteen synthetic peptides incorporating the signaling element exhibit a range of
       affinities for Zn2+ through variation and number of Zn2+ ligands, ligand arrangement
       and the β-turn sequence that acts as a preorganization element between the ligands.
       The stoichiometry of the peptide-Zn2+ complexes is evaluated by several criteria.
       The fluorescence response of these peptides to pH and various important metal ions
       is reported.  Eleven of these sequences form only 1:1 complexes with Zn2+ and their
       affinities range from 10 nM to nearly 1 μM.  When used in concert, these sensors can
       provide Zn2+ concentration information in a valuable range.
IT     607708-61-2P 607708-62-3P
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
         (divalent zinc sensing by chelation-enhanced fluorescence with modular
         and tunable chemosensor scaffold)
REFERENCE COUNT:            49      THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS
                                    RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT


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=> fil caold
FILE 'CAOLD' ENTERED AT 13:54:54 ON 14 JUL 2004
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FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)

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  substance identification.  Title keywords, authors, patent
  assignees, and patent information, e.g., patent numbers, are
  now searchable from 1907-1966.  TIFF images of CA abstracts
  printed between 1907-1966 are available in the PAGE
  display formats.

  This file supports REG1stRY for direct browsing and searching of
  all substance data from the REGISTRY file.  Enter HELP FIRST for
  more information.

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=> => s l15
L17          0 L15

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=> fil reg
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STRUCTURE FILE UPDATES:    13 JUL 2004   HIGHEST RN 709042-93-3
DICTIONARY FILE UPDATES:   13 JUL 2004   HIGHEST RN 709042-93-3

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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L15  ANSWER 1 OF 3  REGISTRY  COPYRIGHT 2004 ACS on STN
RN   639079-38-2  REGISTRY
CN   2-Quinolinepropanoic acid, α-amino-5-[(dimethylamino)sulfonyl]-8-
```

```
     hydroxy-, (αS)- (9CI)  (CA INDEX NAME)
FS   STEREOSEARCH
MF   C14 H17 N3 O5 S
CI   COM
SR   CA
LC   STN Files:   CA, CAPLUS
DT.CA  CAplus document type:  Journal
RL.NP  Roles from non-patents:  ANST (Analytical study); BIOL (Biological
       study)

Absolute stereochemistry.
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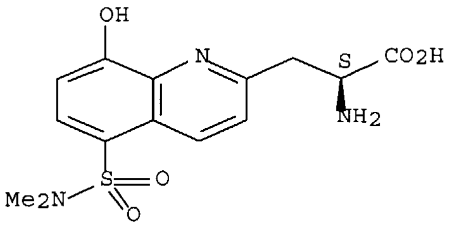

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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

               1 REFERENCES IN FILE CA (1907 TO DATE)
               1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE   1:  140:55461

L15  ANSWER 2 OF 3  REGISTRY  COPYRIGHT 2004 ACS on STN
RN   607708-62-3  REGISTRY
CN   2-Quinolinepropanoic acid, 5-[(dimethylamino)sulfonyl]-α-[[(9H-
     fluoren-9-ylmethoxy)carbonyl]amino]-8-hydroxy-, (αS)- (9CI)  (CA
     INDEX NAME)
FS   STEREOSEARCH
MF   C29 H27 N3 O7 S
SR   CA
LC   STN Files:   CA, CAPLUS
DT.CA  CAplus document type:  Journal
RL.NP  Roles from non-patents:  PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.
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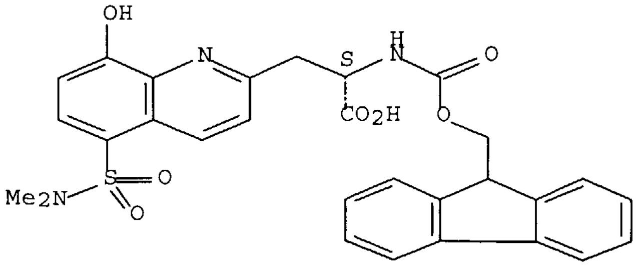

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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

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REFERENCE   1:  139:300801

L15  ANSWER 3 OF 3  REGISTRY  COPYRIGHT 2004 ACS on STN
RN   607708-61-2  REGISTRY
CN   2-Quinolinepropanoic acid, α-amino-5-[(dimethylamino)sulfonyl]-8-
     hydroxy-, monohydrochloride, (αS)- (9CI)  (CA INDEX NAME)
FS   STEREOSEARCH
MF   C14 H17 N3 O5 S . Cl H
SR   CA
LC   STN Files:   CA, CAPLUS
DT.CA  CAplus document type:  Journal
RL.NP  Roles from non-patents:  PREP (Preparation); RACT (Reactant or reagent)
CRN  (639079-38-2)

Absolute stereochemistry.
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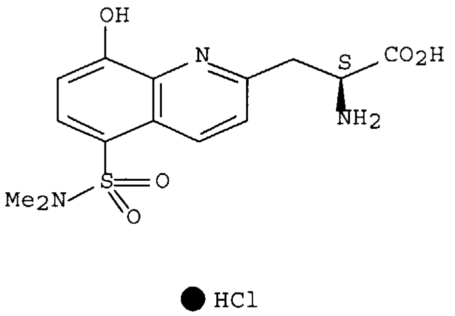

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               1 REFERENCES IN FILE CA (1907 TO DATE)
               1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE   1:  139:300801


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=> fil beil
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FILE RELOADED ON OCTOBER 20, 2002
FILE LAST UPDATED ON JUNE 15, 2004

FILE COVERS 1771 TO 2003.
*** FILE CONTAINS  8,997,153 SUBSTANCES ***

>>> PLEASE NOTE: Reaction data and substance data are stored in
    separate documents and can not be searched together in one
    query.
    Reaction data for BEILSTEIN compounds may be displayed
    immediately with the display codes PRE (preparations) and REA
    (reactions). A substance answer set retrieved after the search
    for a chemical name, a molecular formula or a structure search
    for example can be restricted to compounds with available
    reaction information by concatenation with PRE/FA, REA/FA or
    more general with RX/FA. The BEILSTEIN Registry Number (BRN)
    is the link between a BEILSTEIN compound and belonging reactions.
    For more detailed reaction searches BRNs can be selected from
    substance answer sets and searched in the next step as reaction
    partner BRNs - Reactant (RX.RBRN) or Product BRN (RX.PBRN).
    After a search for reaction details substance documents
    associated with reactants or products may be retrieved by
    searching RX.PBRNs or RX.RBRNs as BRNs. <<<


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* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                        *
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L14                STR
L25              2 SEA FILE=BEILSTEIN SSS FUL L14

100.0% PROCESSED   2057 ITERATIONS                              2 ANSWERS
SEARCH TIME: 00.00.11



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